

A generalized quantum microcanonical ensemble from random matrix product states

Silvano Garnerone¹ and Thiago R. de Oliveira²

¹*Institute for Quantum Computing, University of Waterloo, Waterloo, ON N2L 3G1, Canada*

²*Instituto de Física, Universidade Federal Fluminense,
Av. Gal. Milton Tavares de Souza s/n, Gragoata 24210-346, Niterói, RJ, Brazil*

We propose a tensor network algorithm for the efficient sampling of quantum pure states belonging to a generalized microcanonical ensemble. The algorithm consists in an adaptation of the power method to a recently introduced ensemble of random matrix product states. The microcanonical ensemble that we consider is characterized by the fact that the participating energy eigenstates are not required to have identical statistical weight. To test the method we apply it to the Heisenberg model with an external magnetic field, and we find that the magnetization curves, due to the microcanonical constraint, are qualitatively different from those obtained in the canonical ensemble. Possible future applications include the study of isolated quantum systems evolving after a quantum quench.

PACS numbers: 03.67.-a, 05.30.-d, 75.10.Jm, 75.40.Mg

Introduction.— The problem of representing statistical mechanics ensembles within the more fundamental quantum theory has recently attracted new interest both at the experimental and theoretical level [1–9]. On the experimental side, the ability to isolate quantum systems from their surrounding triggers new questions on quantum thermalization and quantum equilibration dynamics [10]. On the theoretical side, a conceptually new approach based on quantum typicality has emerged as an alternative paradigm for the understanding of quantum statistical mechanics and thermodynamics [7, 8]. Since in quantum mechanics ensembles are represented by density matrices, there are two ways in which they can be obtained: (i) after a partial trace over an environment which is entangled with the system in a global pure state, (ii) averaging over an ensemble of global pure states. The paradigmatic change provided by quantum typicality has taken advantage of the partial trace point of view. Loosely speaking quantum typicality exploits the concentration, around the average value, of some random variable in high dimensional spaces. This can be used for example to justify the occurrence of the canonical ensemble as the reduced density matrix of a typical random pure state [7, 9, 11, 12]. On the other hand, averaging over ensembles of microscopic configurations –point (ii) above– is yet another effective way of representing properties of physical systems [8, 13]. In this work we adopt this second approach, and we provide a tensor network algorithm to sample from a generalized quantum microcanonical ensemble, which differs from the standard microcanonical construction because the requirement for the participating eigenstates to have equal statistical weights is relaxed to a more realistic one [9]. The algorithm consists in an adaptation of the power method to Matrix Product States (MPS), and it exploits statistical properties of a recently introduced ensemble of Random MPS (RMPS) [14, 15], which is the key feature allowing for the computational efficiency of the method. In fact, any alternative

procedure which considers Haar-distributed random pure states would be far less efficient than the present scheme, due to the fact that those states are computationally hard to generate. For the Heisenberg model with an external magnetic field, the qualitative comparison of the results of our simulations with a different approach exploiting Haar-distributed states, also supported by exact calculations [16], corroborates the validity of our method. The introduced computational procedure, and the relative generalized microcanonical ensemble, can also be of relevance in the context of current experimental setups where the quantum system is almost isolated from the environment [1–3].

The RMPS ensemble.— MPS are quantum pure states fully specified by a set $\{A^{\sigma_i}, i = 1, \dots, N\}$ of relatively small dimensional matrices [17]:

$$|\psi\rangle = \sum_{\sigma, i} A_{i_1, i_2}^{\sigma_1} A_{i_2, i_3}^{\sigma_2} \cdots A_{i_{N-2}, i_{N-1}}^{\sigma_{N-1}} A_{i_{N-1}, i_N}^{\sigma_N} \times |\sigma_1 \sigma_2 \cdots \sigma_{N-1} \sigma_N\rangle. \quad (1)$$

Following the standard notation for open-boundary MPS we set the row and column indices $\{i_1, i_N\}$ to 1; while all other indices belong to the set of integers from 1 to χ , the latter being the so called bond-dimension of the MPS. For two levels systems, it follows that an MPS is specified by no more than $2N\chi^2$ numbers which, for χ not too large, is exponentially smaller than the 2^N parameters required by a typical quantum state in the same Hilbert space \mathcal{H} . Indeed, any state can be written as a MPS for χ large enough, but the advantage in using MPSs occurs only when $\chi \sim \text{poly}(N)$. Moreover, MPS are physically relevant since they are good approximations of ground states of short-ranged gapped Hamiltonians, and they can also be used to construct thermal states [13, 17, 18]. With the aim to better understand the usefulness of typicality in quantum statistical mechanics, in [14] an ensemble of random MPS has been proposed sharing some of the statistical features of Haar-distributed random pure

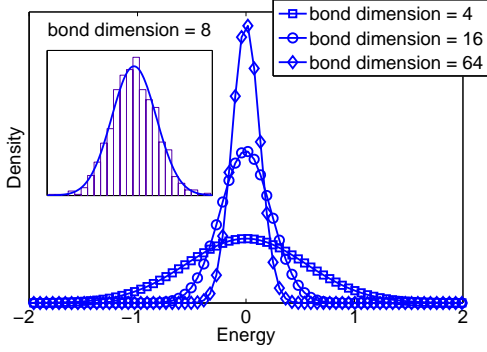


Figure 1. Gaussian fits for the histograms of the expectation values of the transverse field Ising chain with respect to RMPSs. For ease of exposition, in the main figure only the normal fitting curves are shown, while the inset shows a particular histogram with the relative Gaussian fit, for $\chi = 8$. $N = 10$, $\chi = \{4, 16, 64\}$, 1000 realizations.

states. According to the construction presented in [14], a random MPS is defined considering the χ -dimensional matrices $A^{\sigma_i \in \{\uparrow, \downarrow\}}$ as contiguous sub-blocks of a set of N independent Haar-distributed unitaries U_i , each unitary having dimension 2χ (where 2, in general, is the dimension d of the local Hilbert space). In particular, a sufficient condition for the occurrence of typicality in the case of RMPS has been derived in [14], and the exact calculation of the average density matrix of the ensemble has been obtained in [15]. Interestingly enough, the average random MPS coincides with the one obtained from Haar-distributed random states, i.e. it is the maximally mixed state. For an alternative construction of random physical states, though not related to MPS, see also [19–21]. In this letter we show how the RMPS ensemble, together with efficient and relatively simple computational techniques, can be used to sample from a generalized quantum microcanonical ensemble introduced by Reimann [9]. Computational efficiency is inherited from well-known MPS features, while on the statistical side we also exploit some of the properties characterizing the RMPS ensemble. In particular we will use the fact that the average state is equal to the completely mixed state $[\langle \psi | \langle \psi |]_{\text{ave}} = \mathbb{I}/D$, where $|\psi\rangle$ is a random MPS as in Eq. 1, and D is the dimension of \mathcal{H} . One of the implications of the above identity is numerically checked in Fig. 1, where the expectation value of the energy of the transverse field Ising chain is sampled over 1000 realizations of independent random MPS. The results of the simulations confirm that, irrespective of the auxiliary bond dimension χ , the average energy is given by $[\langle \psi | H | \psi \rangle]_{\text{ave}} = \text{Tr} H / D = 0$. Moreover in Fig. 1 one observes that the variance of the distribution depends on χ . We are not able to derive an analytic expression for the second moment of the distribution of RMPS, which would provide the variance in the plots of Fig. 1. Nevertheless, we can check numerically

that the variance of the energy distribution decreases as a power-law with increasing χ , consistently with typicality properties of the ensemble of RMPS [14]. In the case of Haar-distributed random states the characterization of the probability distribution for general observables can be found in [22–28]. We shall now present a computational procedure allowing us to modify the energy distribution from the initial Gaussian centred in 0 to another normal distribution with a desired average value, and whose variance can be reduced with a good degree of control.

A generalized microcanonical ensemble from RMPS.—

Our goal is to modify the initial distribution of Hamiltonian expectation values in such a way that we can arbitrarily choose its center E , and further decrease its variance γ . To accomplish this we use an iterative technique which, starting from an initial RMPS $|\psi\rangle_0$, prepares a final MPS $|\psi\rangle_f$ whose population $p_i \equiv |\langle E_i | \psi \rangle_f|^2$ – with respect to the eigenstates $|E_i\rangle$ of the Hamiltonian – is concentrated on the eigenvectors close in energy to a given value E . The iterative technique is provided by the power method: consider an operator G with maximum eigenvalue λ such that $G|\lambda\rangle = \lambda|\lambda\rangle$. It is easy to show that any initial state $|\psi\rangle_0$, which is not orthogonal to $|\lambda\rangle$, can be used as a starting point to obtain a good approximation to $|\lambda\rangle$, simply iterating the following operation

$$|\psi\rangle_{k+1} = \frac{G|\psi\rangle_k}{\|G|\psi\rangle_k\|_2}, \quad \{k = 0, 1, \dots, f-1\}. \quad (2)$$

For our purposes we set $G = \mathbb{I} - \left(\frac{H-E}{\sigma}\right)^2$, where E is a specified energy value, and σ is a parameter which depends on the spectral range of the local Hamiltonian H , and which has to be chosen so that G is positive semi-definite (a simple estimate is provided by $\sigma = 2N\delta + |E|$, where δ is the greatest absolute value of the Hamiltonian parameters). The power method will bring an initial RMPS $|\psi\rangle_0$ closer to the eigenstate $|E\rangle$, satisfying $H|E\rangle = E|E\rangle$. Indeed, after a number k of iterations $|\psi\rangle_0$ becomes $|\psi\rangle^{(k)} = G^k |\psi\rangle_0 / \|G^k |\psi\rangle_0\|_2$. In the following we provide a simple argument showing that the asymptotic distribution of energies is approximated by a Gaussian centred in E . From the last equation we can write the average density matrix at the k -th iteration as follows: $[\langle \psi | \langle \psi |]_{\text{ave}}^{(k)} \propto [G^k |\psi\rangle \langle \psi| G^k]_{\text{ave}} = G^k [\langle \psi | \langle \psi |]_{\text{ave}} G^k \propto G^{2k}$, where we assumed that with high probability the denominator does not significantly depend on the initial state (as it occurs for Haar-distributed states [9]), and we used the explicit expression for the average state. In the limit of many iterations we can write: $G^{2k} \stackrel{k \gg 1}{\approx} \sum_{|E_i - E| \ll \sigma} \left[1 - \left(\frac{E_i - E}{\sigma}\right)^2\right]^{2k} |E_i\rangle \langle E_i| \sim \sum_{|E_i - E| \ll \sigma} \exp\left[-2k \left(\frac{E_i - E}{\sigma}\right)^2\right] |E_i\rangle \langle E_i|$, where the sum is restricted to those eigenvalues sufficiently close to E .

From the above argument one can derive a polynomial upper-bound (in the size of the system) on the number k of iterations needed in order to have a sufficiently small variance (given by $4\sigma^2/k$): $k \sim \sigma^2 \propto N^2$. For any practical purposes though, our numerical simulations show that already one hundred iterations are sufficient to obtain energy distributions that are concentrated enough, and that can be used to analyse the system. Fig. 2 shows the his-

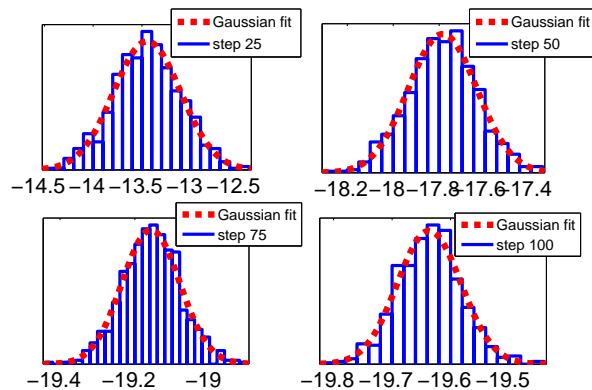


Figure 2. (Color online). Energy histograms and their normal fitting curves at different steps of the power-method iterations. $N = 50$, $\chi = 32$, $E = -20$, 1000 realizations.

tograms of energy values obtained at different steps of the iteration. The simulation confirms that the distribution is indeed a Gaussian whose mean approaches asymptotically the value E , and whose variance decreases algebraically with the number of iterations. The standard Dirac delta function representation of the microcanonical ensemble is approached in the limit of many iterations: $[\langle \psi | \psi \rangle]_{\text{ave}}^{(k)} \xrightarrow{k \rightarrow \infty} \delta(H - E)$. Also, note that Ref. [29] provides a similar but more rigorous derivation of the average state in the context of Haar-distributed random states, showing that indeed the asymptotic final distribution of energies is a Gaussian centred in E . For small systems, using exact diagonalization we observe that at the level of a single RMPS realization the populations p_i of energy eigenstates, which at the beginning is spread over a wide range of energy values, gets more and more concentrated around the chosen E value during the iteration process. This is consistent with the characterization of a generalized microcanonical ensemble, as proposed by Reimann in [9]. In particular, the standard requirement for the microcanonical ensemble, i.e. that *any* participating eigenstate has the *same* probability in the ensemble, is weakened to more general *non-uniform* distributions of eigenstates in the small energy window, like those that we obtain. Reimann argues that these generalized microcanonical energy distributions have to be considered more realistic realizations of the quantum microcanonical ensemble [9]. Indeed, for a not too small system, energy levels are extremely close to each other and experimen-

tally it would be extremely hard to prepare an equal superposition of energy eigenstates. On the other hand it should be much simpler to require a distribution of the energy population with a sharp peak and a small variance (see also [11] and references therein). Note that, in principle, for sufficiently many iterations, one single realization of a random MPS can provide an instance of the quantum microcanonical ensemble, along the lines of the construction presented in [16] for Haar-distributed states. On the other hand, we can exploit the fact that sampling over many RMPS improves the estimate of averaged quantities [30], and we do not need to wait for many iteration steps to terminate as long as we allow for a small finite width in the distribution of energies around their mean value. From this point of view the kind of generalized microcanonical ensemble that we obtain is provided by an ensemble of random pure states which, when expressed in the energy eigenbasis of the Hamiltonian, have support on an energy window whose width can be controlled by the number of iterations, while the number of sampled states controls the accuracy in the estimation of averaged quantities. Moreover, the distribution obtained by sampling the Hamiltonian expectation values is not only meaningful from a statistical mechanics point of view in the regime of many iterations. In fact, the fluctuations in the energy value obtained at finite and not too large k can be interpreted as an energy exchange between the sampled system and a small finite-size environment, weakly interacting with the system. More about this interpretation can be found in [31] where the so-called Gaussian ensemble has been analysed in the context of classical statistical mechanics. For an alternative construction of a generalized quantum microcanonical ensemble see also [32, 33], though in these works there is no constraint on the fact that, in the eigenenergies basis, the states in the ensemble have support only in a small energy window, and in general they do not reproduce the standard canonical ensemble for subsystems.

Application to spin chain Hamiltonians.— In this section we apply the RMPS power method to the Heisenberg model with an external magnetic field: $H = -\sum_{i=1}^N \frac{J}{4} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z) + h \sum_i \sigma_i^z$. To check the validity of the method we compare our results with similar quantities calculated for smaller systems in [16]. We compute the magnetization $m_z \equiv N^{-1} \sum_{i=1}^N [\langle \sigma_i^z \rangle]_{\text{ave}}$ for the ferromagnetic model ($J = 1$), and the correlation function $\phi(j) \equiv N^{-1} \sum_{i=1}^N [\langle \sigma_i^z \sigma_{i+j}^z \rangle]_{\text{ave}}$ for the antiferromagnetic model ($J = -1$). Both Fig. 3 and Fig. 4 show lines labelled by different energy densities $u \equiv E/N$, and each point on the curves is obtained averaging over 200 statistically independent RMPS (we checked that the standard deviations are always very small, of the order of $10^{-3}J$). We note that, from a computational point of view, in order to sample over many random MPS the algorithm can be trivially paral-

lized to efficiently estimate statistical properties of the ensemble. The results of our simulations are qualitatively and quantitatively very similar to those provided in [16], where the authors can also use data obtained from exact calculations in the canonical ensemble which are consistent with their findings. We note that, although our algorithm shares some aspects with the procedure presented in [16], the two computational schemes are substantially different, mainly due to the fact that we make use of an MPS ensemble, allowing us to access much larger spin chains. From a physical point of view it is interesting to note that Fig. 3 shows a non-monotonic behavior of the magnetization with respect to the field, which is quite different from what one obtains in the canonical ensemble at fixed temperature (i.e. monotonic magnetization curves) [34]. Note that this difference between the two ensembles is evident when looking at the ‘global’ behavior of the magnetization curves, while ‘locally’ point-by-point one can always find canonical ensembles (characterized by different temperatures) providing the same results as the generalized microcanonical one [16]. The difference is due to the energy constraint imposed by the quantum microcanonical ensemble, which does not allow the system to explore the same set of states as in the canonical case. In fact there are two main contributions to the Hamiltonian expectation value: one due to the interaction term, the other due to the magnetic field term. For small increasing values of the magnetic field the system can increase its magnetization, while keeping the energy constant, due to the effect of the interaction term which can balance the different energy contribution coming from the magnetic field term (this explains the left side in Fig. 3). On the other hand, when the field is big enough, a further increase in the magnetization can not be compensated by the interaction term, implying that the microcanonical energy constraint would not be satisfied. The only states allowed in this regime are those for which the magnetization decreases with an increasing field. Considering state-of-art experiments with almost isolated quantum systems, it would be interesting to have an experimental confirmation of this behavior in those setup where it is possible to access the energy window of interest, to control the external field and to measure the magnetization. Fig. 4 provides information on the decay of the correlations and on the way in which they can be affected by an external magnetic field. Also in this case our simulations compare well with those provided in Ref. [16].

Conclusions and future directions.— We have presented a tensor network algorithm which can be used to sample states belonging to a given energy window. Statistical properties of the initial ensemble of random MPS, and the exploitation of tensor network structures make the algorithm suitable for the simulation of large one-dimensional systems. This algorithm allows us to test new ideas in the foundations of quantum statistical

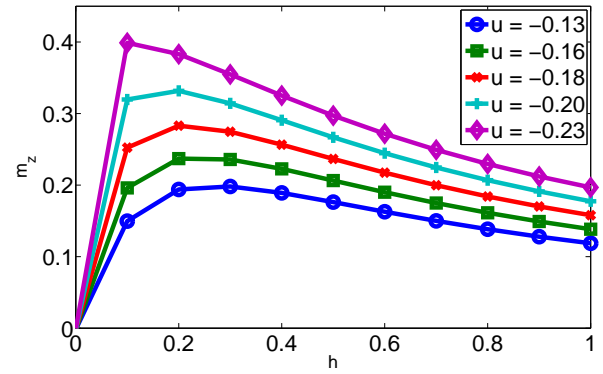


Figure 3. (Color online). Magnetization curves of the ferromagnetic Heisenberg chain with an external field, for different values of the energy density. $N = 50$, $\chi = 16$.

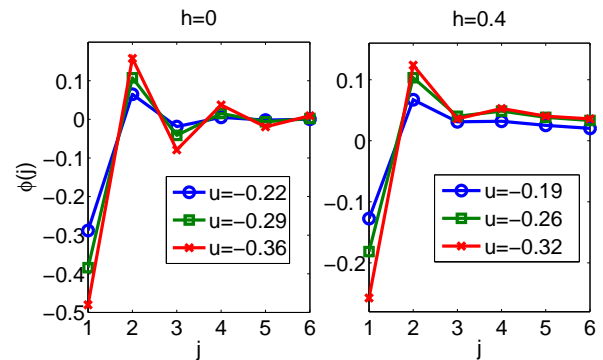


Figure 4. (Color online). Average correlation function of the antiferromagnetic Heisenberg chain with an external field, for different values of the energy density. The figure on the left shows the results with $h = 0$, while the figure on the right shows the results for $h = 0.4$. $N = 50$, $\chi = 16$.

mechanics regarding a generalization of the quantum microcanonical ensemble, as presented in [9]. With respect to this, in the future we plan to study in more details computational aspects connected to quantum typicality in our ensemble of random MPS. Our approach suggests also a new algorithm for the simulation of quantum systems in the canonical ensemble, with some features similar to the algorithm proposed in [13]. In the context of quantum computation it would also be interesting to investigate the computational complexity of a quantum algorithm able to sample from the microcanonical distribution. Along the lines of our construction, one should combine a subroutine implementing a quantum pseudo-random circuit [35] used to generate random quantum states, together with the iterative application of the operator G in Eq.2 using the technique developed in [36]. Alternatively one could think of adapting a similar quantum circuit into the framework of mixed states quantum computation [37, 38].

Acknowledgements. SG is grateful to L. Campos

Venuti, I. Di Marco, S. Haas and P. Zanardi for insightful comments. TRO thanks R. G. Pereira and J. A. H. Neto for useful discussions.

-
- [1] T. Kinoshita, T. Wenger, and D. S. Weiss, *Nature* **440**, 900 (2006).
- [2] S. Hofferberth, I. Lesanovsky, B. Fischer, T. Schumm, and J. Schmiedmayer, *Nature* **449**, 324 (2007).
- [3] I. Bloch, J. Dalibard, and W. Zwerger, *Reviews of Modern Physics* **80**, 885 (2008).
- [4] M. Lewenstein, A. Sanpera, V. Ahufinger, B. Damski, A. Sen, and U. Sen, *Advances in Physics* **56**, 243 (2007).
- [5] J. Gemmer, M. Michel, and G. Mahler, *Lecture Notes in Physics* **657** (2004).
- [6] A. Polkovnikov, K. Sengupta, A. Silva, and M. Vengalattore, *Reviews of Modern Physics* **83**, 863 (2011).
- [7] S. Popescu, A. Short, and A. Winter, *Nature Physics* **2**, 754 (2006).
- [8] S. Goldstein, J. Lebowitz, R. Tumulka, and N. Zanghi, *Journal of statistical physics* **125**, 1193 (2006).
- [9] P. Reimann, *Physical Review Letters* **99**, 160404 (2007).
- [10] M. Rigol, V. Dunjko, and M. Olshanii, *Nature* **452**, 854 (2008).
- [11] S. Goldstein, J. Lebowitz, R. Tumulka, and N. Zanghi, *Physical review letters* **96**, 50403 (2006).
- [12] P. Reimann, *Journal of Statistical Physics* **132**, 921 (2008).
- [13] S. R. White, *Physical Review Letters* **102**, 190601 (2009).
- [14] S. Garnerone, T. De Oliveira, and P. Zanardi, *Physical Review A* **81**, 032336 (2010).
- [15] S. Garnerone, T. De Oliveira, S. Haas, and P. Zanardi, *Physical Review A* **82**, 052312 (2010).
- [16] S. Sugiura and A. Shimizu, *Physical Review Letters* **108**, 240401 (2012).
- [17] U. Schollwöck, *Annals of Physics* **326**, 96 (2011).
- [18] E. Stoudenmire and S. R. White, *New Journal of Physics* **12**, 055026 (2010).
- [19] A. Hamma, S. Santra, and P. Zanardi, *Physical Review Letters* **109**, 40502 (2012).
- [20] A. Hamma, S. Santra, and P. Zanardi, *Phys. Rev. A* **86**, 052324 (2012).
- [21] P. Zanardi, arXiv preprint arXiv:1303.2832 (2013).
- [22] L. Venuti and P. Zanardi, arXiv preprint arXiv:1202.4810 (2012).
- [23] T. Galloway and D. Serre, *Communications on Pure and Applied Mathematics* **65**, 287 (2011).
- [24] Z. Puchał, J. A. Miszcza, P. Gawron, C. F. Dunkl, J. A. Holbrook, and K. Życzkowski, *Journal of Physics A: Mathematical and Theoretical* **45**, 415309 (2012).
- [25] C. F. Dunkl, P. Gawron, J. A. Holbrook, J. A. Miszcza, Z. Puchał, and K. Życzkowski, *Journal of Physics A: Mathematical and Theoretical* **44**, 335301 (2011).
- [26] C. F. Dunkl, P. Gawron, J. A. Holbrook, Z. Puchał, and K. Życzkowski, *Linear Algebra and its Applications* **434**, 2042 (2011).
- [27] D. C. Brody, D. W. Hook, and L. P. Hughston, *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Science* **463**, 2021 (2007).
- [28] D. C. Brody, D. W. Hook, and L. P. Hughston, in *Journal of Physics: Conference Series*, Vol. 67 (IOP Publishing, 2007) p. 012025.
- [29] M. W. Long, P. Prelovek, S. El Shawish, J. Karadamoglou, and X. Zotos, *Physical Review B* **68**, 235106 (2003).
- [30] W. Hoeffding, *Journal of the American Statistical Association* **58**, 13 (1963).
- [31] M. Challa and J. Hetherington, *Physical review letters* **60**, 77 (1988).
- [32] M. Müller, D. Gross, and J. Eisert, *Communications in Mathematical Physics* **303**, 785 (2011).
- [33] B. Fine and F. Hantschel, arXiv preprint arXiv:1010.4673 (2010).
- [34] J. C. Bonner and M. E. Fisher, *Phys. Rev.* **135**, A640 (1964).
- [35] A. W. Harrow and R. A. Low, *Communications in Mathematical Physics* **291**, 257 (2009).
- [36] A. W. Harrow, A. Hassidim, and S. Lloyd, *Phys. Rev. Lett.* **103**, 150502 (2009).
- [37] E. Knill and R. Laflamme, *Phys. Rev. Lett.* **81**, 5672 (1998).
- [38] A. Ambainis, L. J. Schulman, and U. V. Vazirani, in *Proceedings of the thirty-second annual ACM symposium on Theory of computing* (ACM, 2000) pp. 697–704.
- [39] D. Pérez-García, F. Verstraete, M. Wolf, and J. Cirac, *Quantum Information & Computation* **7**, 401 (2007).
- [40] C. Schön, K. Hammerer, M. Wolf, J. Cirac, and E. Solano, *Physical Review A* **75**, 032311 (2007).
- [41] F. Mezzadri, *Notices Am. Math. Soc.* **54**, 592 (2007).
- [42] B. Collins, C. González-Guillén, and D. Perez-Garcia, arXiv preprint arXiv:1201.6324 (2012).

Generation of random MPS

The Hilbert space of a system of N qubits is exponentially big in N , hence typically it would require an exponential number of coefficients to characterize a state in a given basis. Matrix product states provide a solution to this problem, since they allow for a compact description of the states [17, 39]. MPS are represented as linear combinations of basis vectors whose coefficients are given in terms of products of matrices. For a system composed of N particles, with local Hilbert space dimension d , an MPS state can be specified using only a number dN of A^{σ_i} matrices (where $i = 1, \dots, N$), of dimension at most χ (a parameter known as the bond dimension). Thus, the d^N coefficients required for a typical state in the Hilbert space are compressed into a set of at most $dN\chi^2$ numbers, which makes computations much more efficient, but of course also restricts the class of possible states. Fortunately this restricted set can represent good approximations for many interesting states of relevance in condensed matter. More specifically, MPS are able to represent any state whose entanglement obeys the area law or only violates it logarithmic.

With respect to the boundary conditions, there are two different constructions of MPS: with periodic or with

open boundaries. In the first case the state is written as

$$|\psi\rangle = \sum_{\sigma} \text{Tr}[A^{\sigma_1} A^{\sigma_2} \dots A^{\sigma_N}] |\sigma_1 \sigma_2 \dots \sigma_N\rangle,$$

while for open boundaries the first and last matrices are row and column vectors

$$|\psi\rangle = \sum_{\sigma} \langle \phi_L^{\sigma_1} | A^{\sigma_2} \dots A^{\sigma_{N-1}} | \phi_R^{\sigma_N} \rangle |\sigma_1 \sigma_2 \dots \sigma_N\rangle.$$

One can also consider the case where the A matrices are the same at each site, a so-called homogeneous MPS. Together with periodic boundary conditions this also gives a translational invariant state. Note that a general non-homogeneous MPS, with or without open boundaries, can also describe a translational invariant state [39]. There is no unique correspondence between the set of pure MPS states and the set of A matrices: different set of matrices may generate the same MPS. This gauge degree of freedom can be fixed using two canonical forms for the MPS: left-canonical MPS or right-canonical MPS. In the left-canonical form the A matrices satisfy the following condition: $\sum_{\sigma_i} A^{\sigma_i \dagger} A^{\sigma_i} = \mathbb{I}$. In the right-canonical form the A matrices satisfy the following condition: $\sum_{\sigma_i} A^{\sigma_i} A^{\sigma_i \dagger} = \mathbb{I}$. When constructing an MPS in canonical form the boundary sites can violate the above conditions, but this simply means that the state is not normalized and it also provides an efficient way to evaluate its norm [17].

In defining the ensemble of random MPS [14] we took inspiration from the sequential generation of MPS [39, 40], according to which a matrix product state can be seen as the outcome of a sequential interaction of unitary matrices between local physical degrees of freedom and an ancillary space. Along this line a natural way for defining a random MPS starts by considering a random Haar-distributed unitary matrix U [41] of dimension $d\chi$, which can be seen as composed of blocks in the following way (for simplicity we now restrict to the case $d = 2$)

$$U = \begin{bmatrix} M & V \\ N & W \end{bmatrix},$$

where each block has dimension χ . Identifying the block M and N with the two $A^{\sigma_i=1,0}$ matrices associated to a local qubit immediately provides the building block for the construction of a left-canonical random MPS. On the other hand a right-canonical MPS can be obtained by identifying the two $A^{\sigma_i=1,0}$ matrices with M and V . Similar considerations hold for the block column matrices V and W , or for the row column matrices N and W . A non-homogeneous random MPS can be iteratively constructed by sampling from a set of N independent random unitary matrices, each of dimension 2χ . In the case of open boundary conditions the first and last A matrices are simply obtained from random Haar-distributed

vectors. Therefore the ensemble of random MPS generated in this way is appealing for different reasons: it has a natural operational meaning, the state is obtained in a canonical form, and it allows to use properties of the Haar distribution. Typicality and other properties of the ensemble of random MPS have been studied in [14, 15, 42].

Computational cost of the algorithm

Our algorithm is an instance of the simple and widely used power method, an iterative technique which does not require any diagonalization or singular value decomposition. Instead one has to deal only with matrix-vector multiplications, during which an operator G is repeatedly applied to an initial state $|\psi\rangle$.

In order to estimate the computational resources required by our scheme, we start by defining the operations needed in its implementation: generation of a random matrix product state $|\psi\rangle$; construction of the operator G ; application of the operator G to $|\psi\rangle$; if needed the evaluation of some expectation values. Except for the generation of random MPS, all other computational steps are already well discussed in the literature (see for example [17]), and are summarized here just for completeness.

The generation of the initial random MPS has been described in the previous section. To estimate the computational resources, in the worst case, we only need to multiply by N (the length of the chain) the cost of the generation of a random unitary of size $d\chi$, where d is the local Hilbert space dimension (2 in the case of qubits) and χ is the maximum allowed bond-dimension of the MPS. Since χ is at most a polynomial in N , the state can be generated with an amount of resources scaling polynomially in N .

The construction of the operator $G \equiv \mathbb{I} - \left(\frac{H-E}{\sigma}\right)^2$ —where H is the Hamiltonian of the system, while E and σ are two given numbers— involves the Matrix Product Operator (MPO) representation of the identity matrix and of the first and second powers of the Hamiltonian. The MPO representation is the most effective way of dealing with operators in the MPS framework: it simply consists in the generalization to operators of the matrix product decomposition for states (see for example [17] for more details)

$$O = \sum_{\sigma, \sigma'} W^{\sigma_1, \sigma'_1} W^{\sigma_2, \sigma'_2} \dots W^{\sigma_N, \sigma'_N} |\sigma\rangle \langle \sigma'|, \quad (3)$$

where the bond-dimension of the W matrices is typically small (equal to 5 or 9 as we will see). The MPO representation of the identity matrix is very simple, while less trivial is the representation of the Hamiltonian. An efficient way of constructing it is explained in [17] (see page 142). It requires an MPO of bond-dimension 5 for the representation of H , while the cost of the representation

of H^2 can be optimized using a bond-dimension equal to 9. We note that clearly the construction of the operator G has to be done only once at the beginning of the algorithm. Hence the MPO representation of G requires the storage of a number $4N$ of matrices of dimension at most 9 (25 if one does not optimize the construction of H^2).

The third step in the algorithm consists in the application of the MPO G to the MPS $|\psi\rangle$ which, for an MPS of bond-dimension χ and an MPO of bond-dimension χ_W , costs $\mathcal{O}(Nd^2\chi^2\chi_W^2)$. Since G is composed by a linear combination of different MPOs, and since after the application of G to $|\psi\rangle$ the bond-dimension of the state increases by a factor given by the MPO bond-dimension,

we need to compress the resulting state to one with a smaller bond-dimension. This can be done using a variational technique costing at most $\mathcal{O}(N\chi^3\chi_W^3)$ [17].

The above operations can be repeated for the desired number of times during the execution of the power method algorithm, and one can keep track of the expectation values of relevant observables at a cost which is linear in N , at most cubic in χ and at most quadratic in χ_W [17].

To conclude we note that in order to sample many different initial random MPS the algorithm can be trivially parallelized without penalizing the efficiency of the scheme.